UCRL-JC-118431 abs

Abstract Submitted
for the March Meeting of the American Physical Society
San Jose, CA
March 20-24, 1995

Suggested Session Title:
Statistical Mechanics

Sorting Category:
3e

Fluid-Fluid Phase Separations in Nonadditive Hard Sphere Mixtures,* F. H. Ree, Lawrence Livermore National Laboratory, J. Jung and M. S. Jhon, Korea Advanced Institute of Science and Technology -- We examined the phase stability for a system of non-additive hard sphere mixtures with equal diameters, *d*, between like-species and an unequal collision diameter, $d(1+\alpha)$, between unlike species. This was done by refining an earlier[1] analytic equation of state (EOS) [J. Chem. Phys. **100**, 9064 (1994)] within the mixed fluid phase range. The new EOS is based on Monte Carlo data over a wide range of density, composition, and α. It is superior to results derived from available theoretical models. If α is less than 0.026, the fluid phase remains homogenous up to the freezing point. The radial distribution functions, local mole fraction, and coordination numbers exhibit a significant number dependence near the fluid phase boundary, reflecting fluctuations in heterogeneous clusters and sending a precursory signal for an impending phase change.

Prefer
X Standard Session

Francis H. Ree
APS Membership No.: MRE192699
Lawrence Livermore National Lab
P.O. Box 808, L-299
Livermore, CA 94550

*Work performed under the auspices of the US Department of Energy by LLNL under contract no. W-7405-ENG-48.